STN -Structure Search
11/3/05

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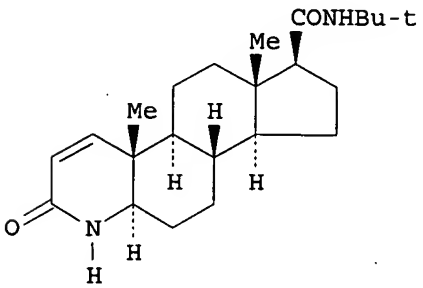
(Inventors)

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:74124 CAPLUS
DOCUMENT NUMBER: 142:156211
TITLE: Method for the preparation of highly pure 1-androstene derivatives with an oxidizing agent while maintaining pH control
INVENTOR(S): Moon, Young Ho; Kim, Dong Jun; Park, Chul-Hyun; Lee, Kyung Ik; Lee, Jae Cheol; Lee, Gwan Sun; Chang, Young-Kil
PATENT ASSIGNEE(S): Hanmi Pharm. Co., Ltd., S. Korea
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005007670	A1	20050127	WO 2004-KR1786	20040719

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: KR 2003-49529 A 20030719
OTHER SOURCE(S): CASREACT 142:156211
GI



I

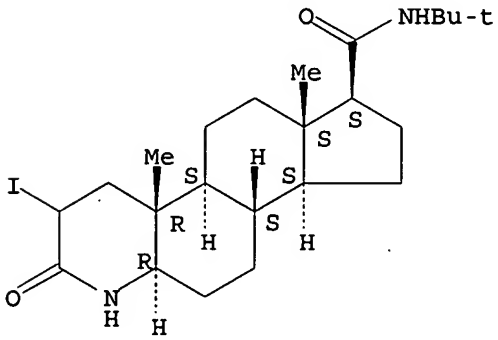
AB A method for preparing a 1-androstene derivative, I, which comprises reacting a 2-iodo-androstane derivative with an oxidizing agent while maintaining the pH of the reaction mixture at a specific range gives the 1-androstene derivative with high purity and yield.

IT **140700-61-4P**
RL: IMF (Industrial manufacture); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(method for the preparation of highly pure 1-androstene derivs. by treating a 2-iodo-androstane derivative with an oxidizing agent while maintaining the pH)

RN 140700-61-4 CAPLUS
CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-

dimethylethyl)hexadecahydro-3-iodo-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

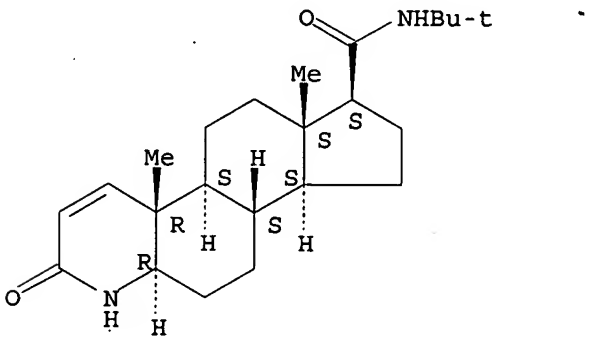
Absolute stereochemistry.



IT **98319-26-7P 164656-23-9P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(method for the preparation of highly pure 1-androstene derivs. by treating a 2-iodo-androstane derivative with an oxidizing agent while maintaining the pH)

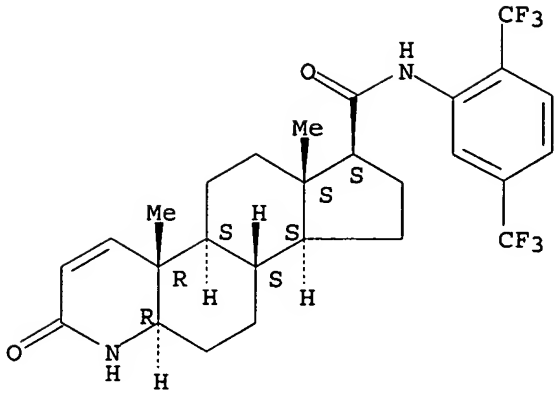
RN 98319-26-7 CAPLUS
CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 164656-23-9 CAPLUS
CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-[2,5-bis(trifluoromethyl)phenyl]-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

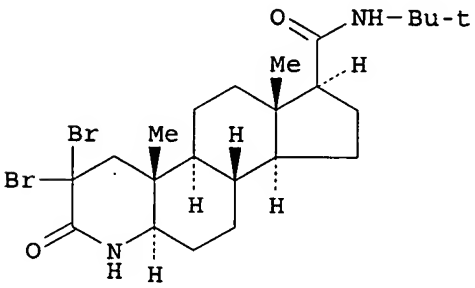


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:399259 CAPLUS
DOCUMENT NUMBER: 140:375356
TITLE: Preparation of 2,2-dibromo-azasteroid and its use for introducing a 1,2-double bond into azasteroids
INVENTOR(S): Slemon, Clarke; Macel, Bob
PATENT ASSIGNEE(S): Torcan Chemical Ltd., Can.
SOURCE: Can. Pat. Appl., 32 pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2271974	AA	20001114	CA 2000-2271974	19990514
PRIORITY APPLN. INFO.:			CA 2000-2271974	19990514

OTHER SOURCE(S): CASREACT 140:375356; MARPAT 140:375356
GI



I

AB A process for introducing a 1,2-double bond into 17β-substituted-3-oxo-4-azasteroids includes the preparation of novel 2,2-dibromo-4-azasteroids by a three step process comprising oxalylation, reaction with excess bromine, and removal of the oxalyl group. This process is preferably carried out at temps. at or above -20°C and results in a high yield of the 2,2-dibromo-4-azasteroid. Thus, dibromodihydrofinasteride I was prepared from dihydrofinasteride. The 2,2-dibromo-4-azasteroid can be converted to the corresponding 17β-substituted-4-aza-5α-androst-

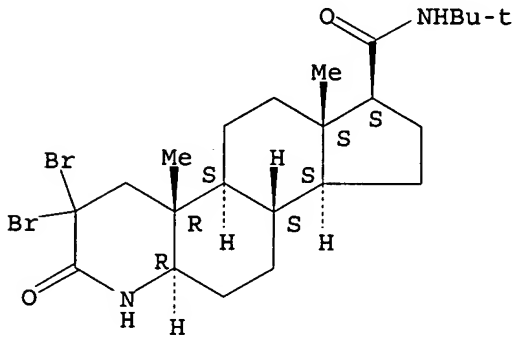
1-ene-3-one, finasteride, by at least two processes, one of which involves correcting the oxidation state at the 2-carbon and then introducing the 1,2-double bond, and the other of which involves introducing the unsatn. to produce a vinyl bromide followed by correcting the oxidation state of the 2-carbon. Preferably, the dibromo compound is reacted with thiophenol to produce a 2-phenylthio intermediate, followed by oxidation of the phenylthio group to a sulfoxide and 1,2-elimination of the sulfoxide group to create the 1,2- double bond.

IT **684215-48-3P**
RL: IMF (Industrial manufacture); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of finasteride via dibromodihydrofinasteride)

RN 684215-48-3 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, 3,3-dibromo-N-(1,1-dimethylethyl)hexadecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

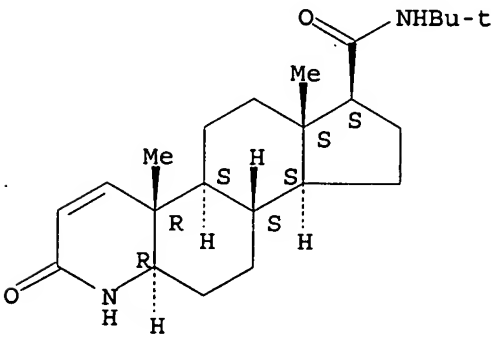


IT **98319-26-7P**, Finasteride
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of finasteride via dibromodihydrofinasteride)

RN 98319-26-7 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:282583 CAPLUS
DOCUMENT NUMBER: 138:287866
TITLE: Process for the preparation of 17β-substituted-3-

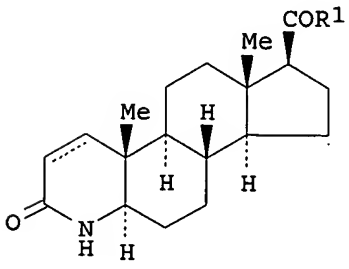
	oxo-Δ1,2-4-azasteroids and intermediates thereof
INVENTOR(S):	Gorgojo Lobato, Jose Maria; Lorente Bonde-Larsen, Antonio; Martin Juarez, Jorge
PATENT ASSIGNEE(S):	Ragactives, S.L., Spain
SOURCE:	PCT Int. Appl., 27 pp.
	CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	Spanish
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

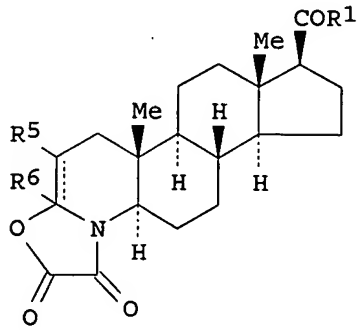
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003029267	A2	20030410	WO 2002-ES453	20020926
WO 2003029267	A3	20030619		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
ES 2185503	A1	20030416	ES 2001-2190	20010929
ES 2185503	B1	20040801		
CA 2461221	AA	20030410	CA 2002-2461221	20020926
EP 1437361	A2	20040714	EP 2002-779579	20020926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005504130	T2	20050210	JP 2003-532513	20020926
US 2004254209	A1	20041216	US 2004-810128	20040326

PRIORITY APPLN. INFO.:	ES 2001-2190	A	20010929
	WO 2002-ES453	W	20020926
OTHER SOURCE(S):	CASREACT 138:287866; MARPAT 138:287866		

GI



I



II

AB The present invention discloses a process for preparing 17β-substituted-3-oxo-Δ1,2-4-azasteroids, such as I [R1 = alkyl, OR2; R2 = alkyl, NR3R4; R3,R4 = H, alkyl; dashed line = double bond], from 17β-substituted-3-oxo-4-azasteroids I [dashed line = single bond]. Thus, I [R1 = NHBu-t; dashed line = single bond] was reacted with oxalyl chloride to provide oxazolidinedione derivative II [R1 = NHBu-t; R5,R6 = H; dashed line = double bond], which upon reaction with 1,3-dibromo-5,5-dimethyl-hydantoin in presence of perchloric acid afford 2-bromo-3-hydroxyoxazolididione derivative II [R1 = NHBu-t; R5 = Br, R6 = OH;

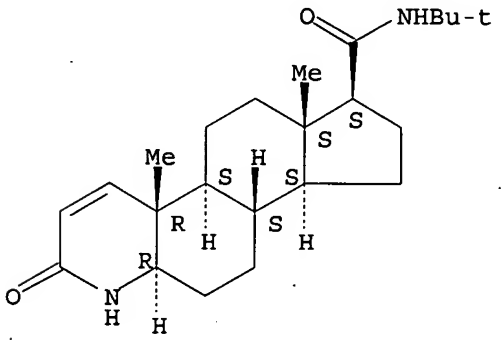
dashed line = single bond (III)]. III was reacted with potassium tert-butoxide in presence of anhydrous DMF to afford I [R1 = NHBu-t; dashed line = double bond]. Some prepared compds. are inhibitors of testosterone-5α-reductase and can be used in the treatment of hyperandrogenic alterations.

IT **98319-26-7P**, Finasteride **140852-02-4P**
507221-54-7P
RL: IMF (Industrial manufacture); **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of 17β-substituted-3-oxo-Δ1,2-4-azasteroids and intermediates thereof)

RN 98319-26-7 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

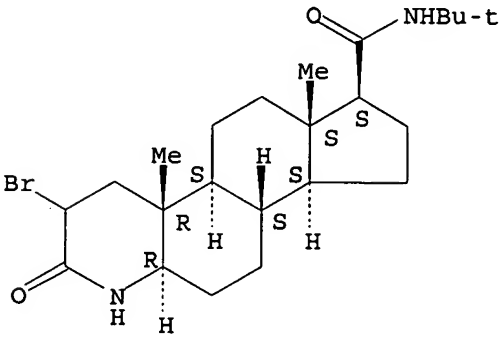
Absolute stereochemistry.



RN 140852-02-4 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, 3-bromo-N-(1,1-dimethylethyl)hexadecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

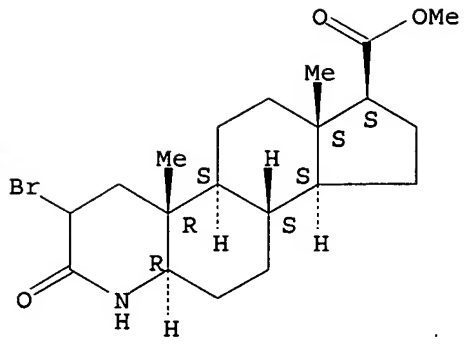
Absolute stereochemistry.



RN 507221-54-7 CAPLUS

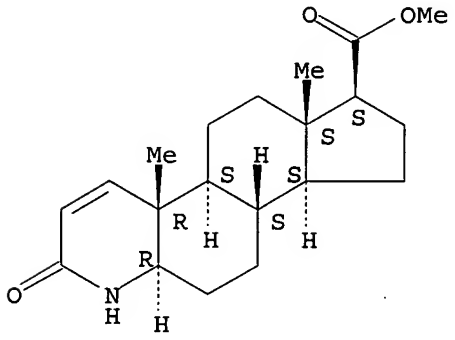
CN 1H-Indeno[5,4-f]quinoline-7-carboxylic acid, 3-bromohexadecahydro-4a,6a-dimethyl-2-oxo-, methyl ester, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **103335-41-7P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of 17β-substituted-3-oxo-Δ1,2-4-azasteroids and intermediates thereof)
RN 103335-41-7 CAPLUS
CN 1H-Indeno[5,4-f]quinoline-7-carboxylic acid, 2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, methyl ester, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:235962 CAPLUS
DOCUMENT NUMBER: 116:235962
TITLE: Process for iodinating or brominating the alpha-methylenic carbon of a secondary amide
INVENTOR(S): King, Anthony On Ping; Abramson, Newton L.; Anderson, Kevin; Shuman, Richard F.; Karady, Sandor
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Eur. Pat. Appl., 11 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

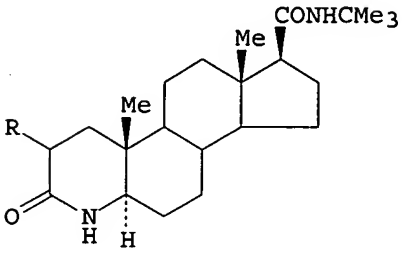
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 473225	A2	19920304	EP 1991-202133	19910821
EP 473225	A3	19931118		
EP 473225	B1	19970709		

R: CH, DE, FR, GB, IT, LI, NL

US 5120847	A	19920609	US 1990-572920	19900827
CA 2049882	AA	19920228	CA 1991-2049882	19910826
CA 2049882	C	20020122		
JP 04261195	A2	19920917	JP 1991-215266	19910827
JP 06049674	B4	19940629		

PRIORITY APPLN. INFO.: US 1990-572920 A 19900827
OTHER SOURCE(S): CASREACT 116:235962; MARPAT 116:235962

GI



I

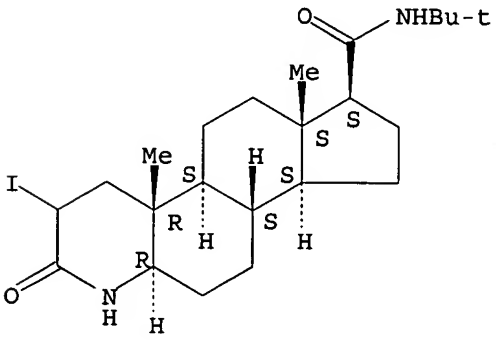
AB The α-methylenic C of a secondary amide is halogenated by Br or iodine in the presence of a trialkylsilyl halide. Thus, androstane I (R = H) was treated with iodine in the presence of Me3SiCl and Me2NCH2CH2NMe2 in PhMe to give I (R = iodo) quant. The latter compound was treated with KOCMe3 in DMF to give 1-androstene.

IT **140700-61-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydroiodination of)

RN 140700-61-4 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)hexadecahydro-3-iodo-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

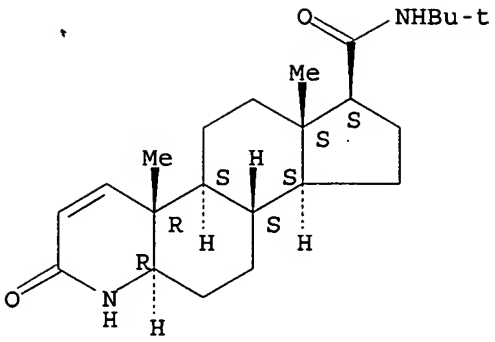


IT **98319-26-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

RN 98319-26-7 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

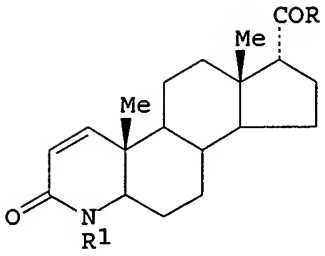
Absolute stereochemistry.



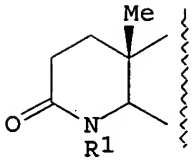
L9 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:472017 CAPLUS
DOCUMENT NUMBER: 115:72017
TITLE: Method for introducing a 1,2 double bond into azasteroids
INVENTOR(S): King, Anthony O.; Weinstock, Leonard M.; Anderson, Kevin R.; Shuman, Richard F.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 428366	A2	19910522	EP 1990-312341	19901113
EP 428366	A3	19920729		
EP 428366	B1	19950920		
R: CH, DE, FR, GB, IT, LI, NL				
US 5021575	A	19910604	US 1989-434663	19891113
CA 2029859	AA	19910514	CA 1990-2029859	19901113
CA 2029859	C	20020514		
JP 03206096	A2	19910909	JP 1990-304208	19901113
JP 06051718	B4	19940706		
EP 655459	A2	19950531	EP 1995-200326	19901113
EP 655459	A3	19960522		
EP 655459	B1	20000503		
R: CH, DE, FR, GB, IT, LI, NL				
LV 12572	B	20010420	LV 2000-117	20000907

PRIORITY APPLN. INFO.: US 1989-434663 A 19891113
EP 1990-312341 A3 19901113
OTHER SOURCE(S): CASREACT 115:72017; MARPAT 115:72017
GI



I



II

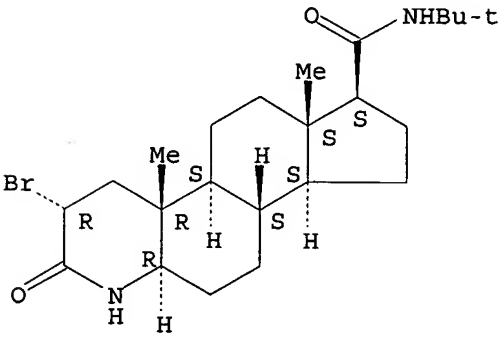
AB 1,2-Unsatd. azasteroids I [R = H, (un)substituted C1-12 alkyl, cycloalkyl, Ph, OH, alkoxy, OCH2Ph, amino; R1 = H, Me, Et] were prepared from saturated derivs. II in a 3-step 1-pot reaction. Thus, II (R = CMe3, R1 = H) was converted to oxazolidinedione derivs. with oxalyl chloride, brominated with Br, treated with MeNHCH2CH2OH to hydrolyze the oxazolidinedione, and dehydrobrominated with Me3COK. The overall yield of I (R = CMe3, R1 = H) was 60.2%.

IT **135252-08-3P 135252-09-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydrobromination of)

RN 135252-08-3 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, 3-bromo-N-(1,1-dimethylethyl)hexadecahydro-4a,6a-dimethyl-2-oxo-, (3R,4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

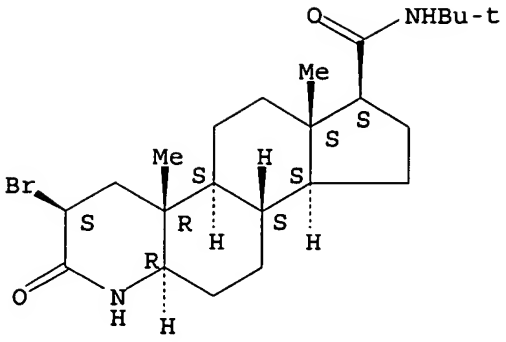
Absolute stereochemistry.



RN 135252-09-4 CAPLUS

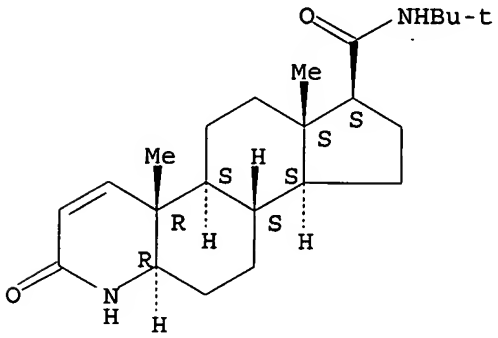
CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, 3-bromo-N-(1,1-dimethylethyl)hexadecahydro-4a,6a-dimethyl-2-oxo-, (3S,4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **98319-26-7P**, MK906
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, from 1,2-dihydro analog)
RN 98319-26-7 CAPLUS
CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



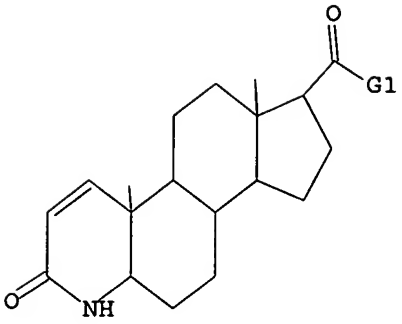
=> d his

(FILE 'HOME' ENTERED AT 09:38:58 ON 03 NOV 2005)

FILE 'REGISTRY' ENTERED AT 09:39:08 ON 03 NOV 2005
L1 STRUCTURE UPLOADED
L2 21 S L1
L3 336 S L1 FULL
L4 STRUCTURE UPLOADED
L5 1 S L4
L6 12 S L4 FULL

FILE 'CAPLUS' ENTERED AT 09:41:20 ON 03 NOV 2005
L7 117 S L3/PREP
L8 5 S L6/RCT
L9 5 S L7 AND L8

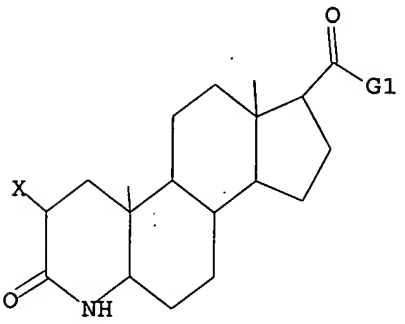
=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> d l4
L4 HAS NO ANSWERS
L4 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

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